

PHASE-MORPHOLOGY AND MOLECULAR STRUCTURE CORRELATIONS IN MODEL FULLERENE-POLYMER NANOCOMPOSITES

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Abstract.

Organic or polymer based photovoltaic devices promise solar technologies that are inexpensive enough to be widely exploited and therefore provide a significant fraction of the future energy needs. There are many promising polymer-fullerene mixtures that are promising materials candidates for achieving high performance device, but their exploitation requires an improved understanding of their structure-property relationships. Of particular relevance is the molecular structural as well as mesoscale phase behaviour.

In order to guide the use of electron acceptor fullerenes in these systems we are using multi-scale molecular modelling coupled with neutron and X-ray scattering to determine the structure behavior of model polymer-fullerene mixtures. Neutron scattering is particularly useful for these types of studies since the fullerene generally have a high scattering contrast with respect to most polymers. This natural contrast, enhanced by careful selective deuteration allows us to carefully probe the atomic and molecular interactions in these complex systems. We are studying model polymer systems to establish fullerene-polymer phase behaviour. To establish how fullerene addition changes polymer phase behaviour, using advanced scattering techniques we are studying phase morphology and molecular structure. Control of morphology development is being examined with particular relevance to solid state processing.